# I U C L I D

# D a t a S e t

| | |
|---|---|
| **Existing Chemical** | ID: 107-45-9 |
| **CAS No.** | 107-45-9 |
| **EC No.** | 203-491-1 |
| **EINECS Name** | 1,1,3,3-tetramethylbutylamine |
| **TSCA Name** | 2-Pentanamine, 2,4,4-trimethyl- |
| **Molecular Formula** | C8H19N |
| **Generic name** | Primene TOA |

**Producer Related Part**

| | |
|---|---|
| **Company:** | Rohm and Haas Company |
| **Creation date:** | 17-MAY-2006 |

**Substance Related Part**

| | |
|---|---|
| **Company:** | Rohm and Haas Company |
| **Creation date:** | 17-MAY-2006 |

| | |
|---|---|
| **Printing date:** | 02-AUG-2006 |
| **Revision date:** | |
| **Date of last Update:** | **02-AUG-2006** |

**Number of Pages:** **28**

| | |
|---|---|
| **Chapter (profile):** | Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10 |
| **Reliability (profile):** | Reliability: without reliability, 1, 2, 3, 4 |
| **Flags (profile):** | Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS |

## 1.0.1 Applicant and Company Information

**Type:** cooperating company
**Name:** Rohm and Haas Company
**Contact Person:** Wendy W. Bingaman **Date:**
**Street:** 727 Norristown Road
**Town:** Spring House, PA
**Country:** United States
**Phone:** 215-619-5531
**Telefax:** 215-619-1657

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

**Type:** cooperating company
**Name:** Rohm and Haas Company
**Contact Person:** Alexis L. Chapman **Date:**
**Street:** 727 Norristown Road
**Town:** Spring House, PA
**Country:** United States
**Phone:** 215-619-5945
**Telefax:** 215-619-1618

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

## 1.0.2 Location of Production Site, Importer or Formulator

**Type:** manufacturer
**Name of Plant:** Houston Plant
**Street:** 1900 Tidal Road
**Town:** 77536 Deer Park, TX
**Country:** United States
**Phone:** 1-281-228-8100

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

## 1.0.3 Identity of Recipients

-

## 1.0.4 Details on Category/Template

-

## 1.1.0 Substance Identification

**Smiles Code:** CC(C)(CC(C)(N)C)C
**Mol. Formula:** C8H19N
**Mol. Weight:** 129.24

**Source:** Rohm and Haas Company, Sprign House, PA, USA
**Reliability:** (1) valid without restriction
17-MAY-2006

17-MAY-2006

## 1.1.1 General Substance Information

**Purity type:** typical for marketed substance
**Substance type:** organic
**Physical status:** liquid
**Purity:** ca. 97 - 100 % v/v
**Colour:** Clear, colorless liquid
**Odour:** Ammonia Odor

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

## 1.1.2 Spectra

-

## 1.2 Synonyms and Tradenames

Primene (TM) is a trademark of Rohm and Haas Company or one of its subsidiaries or affiliates.

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

Primene (TM) TOA Amine

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

## 1.3 Impurities

**Purity type:** typical for marketed substance

**Remark:** Contains small percentages of multiple side reactants.
**Source:** Rohm and Haas Company, Spring House, PA, USA
05-JUL-2006

**Purity type:** typical for marketed substance
**CAS-No:** 7732-18-5
**EC-No:** 231-791-2
**EINECS-Name:** water
**Mol. Formula:** H2O
**Contents:** = .2 - % v/v

**Source:** Rohm and Haas Company, Spring House, PA, USA
05-JUL-2006

## 1.4 Additives

**Remark:** Not applicable
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (1) valid without restriction
14-JUN-2006

## 1.5 Total Quantity

**Quantity:** > 700 tonnes produced in 2005

**Source:** Rohm and Haas Company, Spring House, PA, USA
22-JUN-2006

## 1.6.1 Labelling

**Labelling:** as in Directive 67/548/EEC
**Symbols:** (C) corrosive
(Xn) harmful
**R-Phrases:** (10) Flammable
(22) Harmful if swallowed
(34) Causes burns
**S-Phrases:** (26) In case of contact with eyes, rinse immediately with plenty of water and seek medical advice
(36/37/39) Wear suitable protective clothing, gloves and eye/face protection
(45) In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible)

14-JUN-2006

## 1.6.2 Classification

**Classified:** as in Directive 67/548/EEC
**Class of danger:** harmful
**R-Phrases:** (10) Flammable
(22) Harmful if swallowed
(34) Causes burns

07-JUN-2006

## 1.6.3 Packaging

**Memo:** Packaged in either tank trucks, drums, pails, or small samples.

**Source:** Rohm and Hass Company, Spring House, PA, USA
07-JUN-2006

## 1.7 Use Pattern

**Type:** industrial
**Category:** other: Additive for petroleum products, corrosion inhibitor, rubber, coating resin, agricultural chemicals, pharmaceuticals, polyolefins, surfactants, heavy metal recovery

17-MAY-2006

## 1.7.1 Detailed Use Pattern

**Industry category:** 15/0 other
**Use category:** 55/0 other
**Extra details on use category:** No extra details necessary
No extra details necessary
**Emission scenario document:** not available

**Remark:** Fuel and lubricants, agricultural, pharmaceutcal, metals
17-MAY-2006

## 1.7.2 Methods of Manufacture

**Type:** Production

**Remark:** Test substance is manufactured in batch operations in kettles. All the product is hard-piped to temporary storage tank.
**Source:** Rohm and Haas Company, Spring House, PA, USA
05-JUL-2006

## 1.8 Regulatory Measures

-

### 1.8.1 Occupational Exposure Limit Values

**Type of limit:** other: Rohm and Haas Company
**Limit value:** 3 other: ppm
**Short term exposure**
**Limit value:** 9 other: ppm

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

### 1.8.2 Acceptable Residues Levels

-

### 1.8.3 Water Pollution

-

### 1.8.4 Major Accident Hazards

**Legislation:** other

**Remark:** Evacuate the spill area. Remove all sources of ignition. Floor may be slippery, use care to
avoid falling. Contain spills immediately with inert materials (e.g. sand, earth). Allow material to solidify and transfer solid material to separate suitable containers for recovery or disposal.
WARNING: KEEP SPILLS AND CLEANING RUNOFFS OUT OF MUNICIPAL SEWERS AND OPEN BODIES OF WATER.
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (1) valid without restriction
17-MAY-2006

### 1.8.5 Air Pollution

-

## 1.8.6 Listings e.g. Chemical Inventories

**Type:** EINECS
**Additional Info:** This product is also listed on the following countries product inventory:
Canada
China
Europe Union
Japan
Korea
Philippines

**Source:** Rohm and Haas Company, Spring House, PA, USA
14-JUN-2006

**Type:** TSCA

**Source:** Rohm and Haas Company, Spring House, PA, USA
14-JUN-2006

## 1.9.1 Degradation/Transformation Products

**Type:** degradation product

**Remark:** This material is considered stable under specified conditions of storage, shipment and/or use. There are no known hazardous decomposition products for this material. Product will not undergo polymerization.
17-MAY-2006

## 1.9.2 Components

-

## 1.10 Source of Exposure

**Source of exposure:** Human: exposure by production
**Exposure to the:** Substance

**Remark:** Eyes: Material can cause the following: corrosion to eyes; may cause permanent eye injury.
Skin: Material can cause the following: corrosion to the skin.
Ingestion: Harmful if swallowed.
Inhalation: Inhalation of vapor or mist can cause the following: irritation of the nose, throat and lungs, nausea, vomiting, pulmonary edema.

**Source:** Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

## 1.11 Additional Remarks

-

## 1.12 Last Literature Search

-

## 1.13 Reviews

-

## 2.1 Melting Point

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## 2.2 Boiling Point

-

## 2.3 Density

**Type:** density
**Value:** = .7698 g/cm³

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Value was measured with the Anton-Paar DMA-46 densitometer. Samples were measured in duplicate.
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (2) valid with restrictions
No data on whether test was conducted in compliance with GLP, but test was conducted by recognized scientific standards.
**Flag:** Critical study for SIDS endpoint
17-MAY-2006

(9)

## 2.3.1 Granulometry

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## 2.4 Vapour Pressure

-

## 2.5 Partition Coefficient

**Partition Coeff.:** octanol-water
**log Pow:** ca. 1.09

**Method:** other (measured)
**GLP:** no

**Method:** Shake Flask Method
**Result:** 1.09 +/- 0.20
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
17-MAY-2006

(7)

## 2.6.1 Solubility in different media

-

## 2.6.2 Surface Tension

**Test type:** other
**Value:** = 28 mN/m

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Value was measured on the Fisher Surface Tensiometer, Model 20. Two measurements were performed and the value is an average. The instrument was calibrated using hexane. The values obtained were within 2 dynes/cm from theoretical as given in the CRC handbook.
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (2) valid with restrictions
No data on whether test was conducted in compliance with GLP, but test was conducted by recognized scientific standards.
**Flag:** Critical study for SIDS endpoint
22-MAY-2006 (9)

## 2.7 Flash Point

**Value:** = 15.6 degree C
**Type:** closed cup

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Value was measured using Pensky-Martens closed cup.
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (2) valid with restrictions
No data on whether test was conducted in compliance with GLP, but test was conducted by recognized scientific standards.
**Flag:** Critical study for SIDS endpoint
17-MAY-2006 (9)

## 2.8 Auto Flammability

-

## 2.9 Flammability

-

## 2.10 Explosive Properties

-

## 2.11 Oxidizing Properties

-

## 2.12 Dissociation Constant

**Method:** other
**GLP:** no data
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Potentiometric titration in non-aqueous solvent was used. Using 75/25 isopropanol/octane solvent with 0.1N HCl in isopropanol as titrant, the Half Neutralization Potential (HNP) was determined. The HNP is the potential that develops when equimolar concentrations of nonionized acid and its derived ionized species are present. From this, the pKa value was estimated.

The titrator used was a Radiometer Titralab, equipped with a VIT90 Mark I controller, a SAM90 sample station and an ABU93 buret station. A standard glass electrode and a LiCl reference electrode were used for the titrations.

**Remark:** Due to poor solubility, titration directly in water to determine pKa value was not possible. Value was estimated from HNP.
**Result:** 10.5
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (2) valid with restrictions
**Flag:** Critical study for SIDS endpoint
22-MAY-2006 (4)

## 2.13 Viscosity

-

## 2.14 Additional Remarks

**Memo:** Pour Point

**Method:** ASTM D-97
**Result:** Fluid at -65C
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** As prescribed by 1.1-1.4
**Reliability:** (2) valid with restrictions
17-MAY-2006 (9)

17-MAY-2006

## 3.1.1 Photodegradation

**Type:** other: AOPWIN estimation of hydroxyl radical reaction

**Method:** other (calculated)
**GLP:** no
**Test substance:** other TS

**Method:** AOPWIN v1.91
**Remark:** For hydroxyl radical reactions AOPWIN estimated the hydrogen abstraction rate constant to be 2.25E-12 cm3/molecule-sec. The reaction rate with N, S, and -OH was estimated to be 21.0E-12 cm3/molecule-sec. The overall OH radical rate constant was estimated to be 23.25E-12 cm3/molecule-sec. The estimated half-life equaled 5.52 hours assuming a 12 hour day and 1.5E06 OH/cm3. The model was unable to estimate ozone reaction kinetics because no structurally similar molecules were within the database.
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylamine [CAS No. 107-45-9]; SMILES: CC(C)(CC(C(N)C)C
**Reliability:** (2) valid with restrictions
Value(s) derived using accepted calculation method/software.
22-MAY-2006 (5)

## 3.1.2 Stability in Water

**Method:** other (calculated)
**GLP:** no
**Test substance:** other TS

**Method:** HYDROWIN v1.67
**Remark:** HYDROWIN was unable to estimate hydrolysis rate constant because no similar chemical structures are in the database.
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylamine [CAS No. 107-45-9]; SMILES: CC(C)(CC(C)(N)C)C
**Reliability:** (2) valid with restrictions
Value(s) derived using accepted calculation method/software.
22-MAY-2006 (5)

## 3.1.3 Stability in Soil

-

## 3.2.1 Monitoring Data (Environment)

-

## 3.2.2 Field Studies

-

## 3.3.1 Transport between Environmental Compartments

**Type:** other: Fugacity Model Level I and III
**Media:** other: air, water, soil, sediment
**Method:** other
**Air:** 66.1 % **(Fugacity Model Level I)**
**Water:** 25.3 % **(Fugacity Model Level I)**
**Soil:** 8.5 % **(Fugacity Model Level I)**
**Biota:** 79.1 % **(Fugacity Model Level II/III)**
**Soil:** .0004 % **(Fugacity Model Level II/III)**

**Remark:** Default values were assumed for environmental compartment descriptions, dimensions, and advective and dispersive properties.
Chemical-specific physical properties (at 25 deg. C) used as model input parameters were:

Molecular weight: 129.25
Water Solubility: 10670 (mg/L)
Vapor pressure: 8.03 mm Hg, 1070.58 Pa (estimated using MPBPWIN)
Log Kow: 2.58 (estimated using KOWWIN)
Melting Point: -20.02 (estimated using MPBPWIN)
Half-lives (h):
Air: 11
Water: 900
Soil: 1.8E03
Sediment: 8.1E03
Half-lives were calculated by the model based on the properties of the test substance.

**Result:** Level I

| Compartment | Mass (percent) | Half-life (hr) |
|---|---|---|
| Air | 66.1 | 11 |
| Water | 25.3 | 900 |
| Soil | 8.50 | 1.8E03 |
| Sediment | 0.189 | 8.1E03 |

Level III

| Compartment | Mass (percent) |
|---|---|
| Air | 1.02 |
| Water | 19.7 |
| Water: Fish | 3.74E-04 |
| Soil | 79.1 |
| Sediment | 0.187 |

**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylamine [CAS No. 107-45-9]; SMILES: CC(C)(CC(C)(N)C)C
**Reliability:** (2) valid with restrictions
Value(s) derived using accepted calculation method/software.

22-MAY-2006 (5)

## 3.3.2 Distribution

-

## 3.4 Mode of Degradation in Actual Use

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## 3.5 Biodegradation

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## 3.6 BOD5, COD or BOD5/COD Ratio

-

## 3.7 Bioaccumulation

-

## 3.8 Additional Remarks

-

## AQUATIC ORGANISMS

### 4.1 Acute/Prolonged Toxicity to Fish
-

### 4.2 Acute Toxicity to Aquatic Invertebrates
-

### 4.3 Toxicity to Aquatic Plants e.g. Algae
-

### 4.4 Toxicity to Microorganisms e.g. Bacteria
-

### 4.5 Chronic Toxicity to Aquatic Organisms

### 4.5.1 Chronic Toxicity to Fish
-

### 4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

## TERRESTRIAL ORGANISMS

### 4.6.1 Toxicity to Sediment Dwelling Organisms
-

### 4.6.2 Toxicity to Terrestrial Plants
-

### 4.6.3 Toxicity to Soil Dwelling Organisms
-

### 4.6.4 Toxicity to other Non-Mamm. Terrestrial Species
-

### 4.7 Biological Effects Monitoring
-

### 4.8 Biotransformation and Kinetics
-

## 4.9 Additional Remarks

-

## 5.0 Toxicokinetics, Metabolism and Distribution

-

## 5.1 Acute Toxicity

### 5.1.1 Acute Oral Toxicity

| | |
|---|---|
| **Type:** | LD50 |
| **Species:** | rat |
| **Strain:** | other: Crl:CD BR |
| **Sex:** | male/female |
| **No. of Animals:** | 12 |
| **Vehicle:** | other: none |
| **Doses:** | 50, 150, 200, 500 and 2000 mg/kg bw |
| **Value:** | = 217.7 mg/kg bw |
| **Method:** | OECD Guide-line 401 "Acute Oral Toxicity" |
| **Year:** | 1991 |
| **GLP:** | yes |
| **Test substance:** | as prescribed by 1.1 - 1.4 |

**Method:**

Groups of 12 rats (6/sex) were quarantined for approximately one week, then administered the test substance at dose levels of 50, 150, 200, 500 and 2000 mg/kg. The initial body weight ranges reported were 186 to 215 g for males and 186 to 214 g for females.

The test substance was delivered orally as a single gavage dose undiluted. Rats were fasted overnight prior to dosing. All rats had free access to filtered tap water and feed (Purina Certified Rodent Chow). Animals were housed 2 or 3 per cage and maintained at a temperature of 24oC and a relative humidity range of 40 to 65%. All animals were observed for signs of ill health, or reaction to treatment at 1, 2 and 4 hr after dosing and once daily thereafter for 14 days, and were necropsied following death, as it occurred, or at the end of the observation period.

**Result:**

LD50 values were calculated from the logarithm of the doses and the incidences of mortality using a SAS PROBIT procedure based on the method of D.J. Finney (1971).

Mortality (number of dead /number of animals tested): Dose 50, 150, 200, 500, 2000 mg/kg; Males 1/6, 2/6, 2/6, 6/6, 6/6, respectively; Females 1/6, 0/6, 3/6, 4/5, 6/6, respectively; Combined 2/12, 2/12, 5/12, 10/11, 12/12, respectively.

The LD50 was calculated on the combined mortality incidence data. The acute oral LD50 in male and female rats (combined) was 217.7 mg/kg, with 95% confidence limits of 142.9 and 352.3 mg/kg.

Numerous clinical signs were observed in all doses. These signs included, but were not limited to, ataxia, circling, disoriented behavior, gasping, lacrimation, passiveness, ptosis, tremors and wheezing. Signs found in decedents only were abdominal breathing, arched back, cage biting, emaciation, labored breathing, lethargy and prostration.

Necropsy of decedents revealed the following gross changes related to test substance: black foci on stomach mucosa, clear fluid, mucous-like material and black material (viscera autolyzed) in stomach, distention of intestines and stomach, intestines (including cecum) filled with air, matted fur on muzzle, mucous material in stomach, tan and red staining of the muzzle, red stained eyes, reddened lungs, intestines and cecum, severe reddening of the stomach, tan and/or yellow-stained anogenital area. However, necropsy of the survivors revealed no gross changes related to the test substance.

**Source:** Rohm and Haas Company, Spring House, PA, USA
**Reliability:** (1) valid without restriction
**Flag:** Critical study for SIDS endpoint
02-AUG-2006 (1)

**Type:** other
**Species:** rat

**GLP:** no
**Test substance:** other TS

**Result:** Toxic
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylamine, clear liquid, purity not reported
**Reliability:** (4) not assignable
22-MAY-2006 (6)

## 5.1.2 Acute Inhalation Toxicity

**Type:** other
**Species:** rat

**GLP:** no
**Test substance:** other TS

**Result:** Toxic

All rats dead within 15 minutes.
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylamine, clear liquid, purity not reported
**Reliability:** (4) not assignable
22-MAY-2006 (6)

## 5.1.3 Acute Dermal Toxicity

**Type:** other
**Species:** rabbit

**GLP:** no
**Test substance:** other TS

**Result:** Essentially non-toxic
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylamine, clear liquid, purity not reported
**Reliability:** (4) not assignable
22-MAY-2006

(6)

## 5.1.4 Acute Toxicity, other Routes

-

## 5.2 Corrosiveness and Irritation

## 5.2.1 Skin Irritation

**Species:** rabbit
**Exposure:** Occlusive
**Exposure Time:** 4 hour(s)
**No. of Animals:** 6
**Vehicle:** other: none
**Result:** corrosive

**Method:** OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Occlusive patch test. 0.5 mL applied topically to the shaved intact skin of six New Zealand White rabbits. The application sites were occluded for 4 hours. Skin irritation was evaluated according to the Draize criteria at approximately 1, 24, 48 and 72 hours and 7 and 14 days after patch removal.

**Result:** No mortality or clinical signs were observed. Severe erythema and severe edema were observed at 1 hour. Edema was no longer evident by 72 hours; however, severe erythema continued through to day 14 of the study. Beginning at 24 hours, eschar or concave eschar was observed. On day 14, concave eschar, peripheral scar formation and deep narcosis were observed. The 72 hour Mean Irritation Score (MIS) was 4.0. On day 14, it was concluded that there was irreversible destruction of dermal tissue.

**Source:** Rohm and Haas Company, Spring House, PA, USa
**Reliability:** (1) valid without restriction
22-MAY-2006

(3)

**GLP:** no
**Test substance:** other TS

**Result:** Score 4.7
Not a primary skin irritant, however, test material would be considered a moderate irritant.
**Source:** Rohm and Haas Company, SPring House, PA, USA
**Test substance:** t_octylamine, clear liquid, purity not reported
**Reliability:** (4) not assignable
22-MAY-2006 (6)

## 5.2.2 Eye Irritation

**Test substance:** as prescribed by 1.1 - 1.4

**Remark:** Because t-Octylamine produced corrosive effects to the skin of rabbits, it was determined that the sample be categorized as corrosive to the eyes of rabbits.

Present animal testing guidelines indicate that (i) materials which have demonstrated definitive corrosion or severe irritation in a skin irritation study need not be further tested for eye irritation, and (ii) it may be presumed that substances will produce similarly severe effects in the eyes.
**Source:** Rohm and Haas Company, Spring House, PA, USA
22-MAY-2006 (2)

**Species:** rabbit

**GLP:** no
**Test substance:** other TS

**Result:** Essentially non-toxic
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylaime, clear liquid, purity not reported
**Reliability:** (4) not assignable
22-MAY-2006 (6)

**GLP:** no
**Test substance:** other TS

**Result:** Marked eye irritant
**Source:** Rohm and Haas Company, Spring House, PA, USA
**Test substance:** t-Octylamine, clear liquid, purity not reported
**Reliability:** (4) not assignable
22-MAY-2006 (6)

## 5.3 Sensitization

-

## 5.4 Repeated Dose Toxicity

-

## 5.5 Genetic Toxicity 'in Vitro'

**Type:** Ames test
**System of testing:** Salmonella typhimurium strains TA1535, TA1537, TA98, TA100
**Concentration:** 50, 200, 500, 2000 and 5000 ug/plate
**Metabolic activation:** with and without
**Result:** negative

**Method:** OECD Guide-line 471
**Year:** 1995
**GLP:** yes
**Test substance:** as prescribed by 1.1 - 1.4

**Method:** Strains of Salmonella typhimurium used for this study included: TA98, TA100, TA1535 and TA1537 obtained from Dr. B. Ames, University of California, Berkeley. Strains were characterized for nutritional requirements, crystal violet sensitivity and ampicillin resistance no more than 6 months prior to initiation of the study. The solvent for the test article and the positive control articles (with the exception of sodium azide and 9-aminoacridine) was dimethyl sulfoxide (DMSO). The solvent for sodium azide was distilled water. The solvent for 9-aminoacridine was 95% ethanol.

The positive control, in the presence of metabolic activation, was 2 ug/plate 2-anthramine, for all four strains. In the absence of metabolic activation, the positive controls were 3 ug/plate 2-nitrofluorene for strain TA98; 2 ug/plate sodium azide for strains TA100 and TA1535; and 100 ug/plate 9-aminoacridine for strain TA1537.

The S-9 used for metabolic activation was obtained from rats induced with Aroclor 1254.

The test article was evaluated for mutagenic activity at concentrations ranging from 50 to 5000 ug/plate, with and without metabolic activation, in Salmonella strains TA98, TA100, TA1535 and TA1537. Control plates were run to check for sterility, determine the background reversion rate, and measure the response of each tester strain to a positive control compound.

For the activated portion of the assay the following were added, in order, to sterile test tubes: 2 mL of top agar, 0.1 mL of the bacteria inoculum, 0.1 mL of the appropriate concentration of test compound, and 0.5 mL of phosphate buffer mix (with S-9 and NADP). For the non-activated portion of the assay, the above procedure was followed, except that

the 0.5 mL of phosphate buffer mix (without S-9 or NADP) was added to the tubes directly after addition of the top agar. Each test article concentration was tested in triplicate, in minimal plates (minimal-glucose agar medium). The controls were tested in six replicates in minimal plates. The contents of the tubes were mixed and poured onto petri dishes containing approximately 19 mL of the appropriate agar. Plates were allowed to set for several minutes then placed in covered plastic boxes and incubated at 37 (+ 1) degrees Celsius for approximately 72 hours prior to colony counting.

Following the incubation period, sterility plates were checked for contamination. Following the sterility check, the number of colonies on each plate was determined. The mean and standard deviation for each concentration was calculated. Background growth was checked for each experimental point to observe any toxic response.

A mutagenicity assay is considered valid if the following conditions are met. First, the spontaneous reversion rate, with and without metabolic activation, must be reasonably consistent with the expected range for the strain being used. Second, the positive control materials must elicit a positive response. And third, the strains must maintain characteristics.

A test article is considered positive if it elicits in independent assays a number of revertants per plate at least 2 times that observed in the solvent control (background). A response that does not meet this criteria but elicits a potential biologically significant is considered an equivocal response and requires further evaluation.

A test article is considered negative if the criteria for a positive assay were not met and the test article was tested up to either 5000 ug/plate, the limit of solubility, or the limit of toxicity. Toxicity is defined as the elimination of a uniform background lawn.

**Result:** The test article was evaluated at 50, 200, 500, 2000 and 5000 ug/plate in the presence and absence of S-9.

The study was designed to evaluate the mutagenic potential of the test article up to the limits of solubility, toxicity or 5000 ug/plate (whichever was lower). A contaminant was observed in TA98 and TA1537 in several plates at various dose levels. The contamination was minimal and did not interfere with scoring. A mutagenic response was not detected in any of the four tester strains (TA98, TA100, TA1535 and TA1537) in any of the experiments conducted.

Under the conditions of this study, the test substance was not mutagenic in the Salmonella gene mutation assay.

**Source:** Rohm and Haas Company, Spring House, PA, USA

**Reliability:** (1) valid without restriction

**Flag:** Critical study for SIDS endpoint
22-MAY-2006 (8)

22-MAY-2006

## 5.6 Genetic Toxicity 'in Vivo'

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## 5.7 Carcinogenicity

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## 5.8.1 Toxicity to Fertility

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## 5.8.2 Developmental Toxicity/Teratogenicity

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## 5.8.3 Toxicity to Reproduction, Other Studies

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## 5.9 Specific Investigations

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## 5.10 Exposure Experience

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## 5.11 Additional Remarks

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## 6.1 Analytical Methods

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## 6.2 Detection and Identification

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## 7.1 Function

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## 7.2 Effects on Organisms to be Controlled

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## 7.3 Organisms to be Protected

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## 7.4 User

-

## 7.5 Resistance

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## 8.1 Methods Handling and Storing

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## 8.2 Fire Guidance

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## 8.3 Emergency Measures

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## 8.4 Possib. of Rendering Subst. Harmless

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## 8.5 Waste Management

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## 8.6 Side-effects Detection

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## 8.7 Substance Registered as Dangerous for Ground Water

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## 8.8 Reactivity Towards Container Material

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(1) Bernacki, Jr., HJ and JD Hamilton. 1991. t-Octylamine Acute Oral Toxicity Study in Male and Female Rats. Study conducted at Rohm and Haas Co., Rohm and Haas Toxicology Department Report No. 91R-061, dated July 22, 1991.

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(4) Callan, CR. (1995). pKa Measurements of Primene Products and other Primary Amines using Potentiometric Titration in Non-Aqueous Solvent. Study was conducted at Rohm and Haas Co., Rohm and Haas Analytical Report No. 58-95-041TR, dated February 08, 1995.

(5) Carbone, J.P. (2006). PrimeneTM TOA Amine Quantitative Structure Activity Relationship Modeling. Toxicology Department Memo 06M-020. Rohm and Haas Company, Philadelphia, PA.

(6) Dean, WP and EI Goldenthal. 1973. OSHA Toxicity Screening Tests for Rohm and Haas Company. Study conducted at International Research and Development Corporation, Mattawan, MI, Rohm and Haas Toxicology Department No. 73RC-1091, dated July 31, 1973.

(7) Hafer, JH. (1993). Determination of Octanol/Water Partition Coefficient for Primene TOA by the Shake Flask Method. Study conducted at Rohm and Haas Co., Rohm and Haas Co. Analytical Report No. 13-93-174, dated November 11, 1993.

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(9) Thompson, WA. (1994). Summary of the Physical Properties for the Primene Products. Study conducted at Rohm and HaasCo., Rohm and Haas Co. Analytical Report No. 58-94-133TR, dated June 08, 1994.

## 10.1 End Point Summary

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## 10.2 Hazard Summary

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## 10.3 Risk Assessment

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